

Supplementary data for the article:

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Supplementary Information

C–H/O interactions of nucleic bases with water molecule. Crystallographic and quantum chemical study.

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INFLUENCE OF COUNTER ANIONS/CATIONS COMPOSING OF THE UNIT CELL

In cases where nucleic bases are positively charged (nitrogen atoms are protonated), they form hydrogen bonds between N-H groups and counter anions. In that way, N-H groups are not available for interactions with water molecules and water molecules form C-H/O interaction.

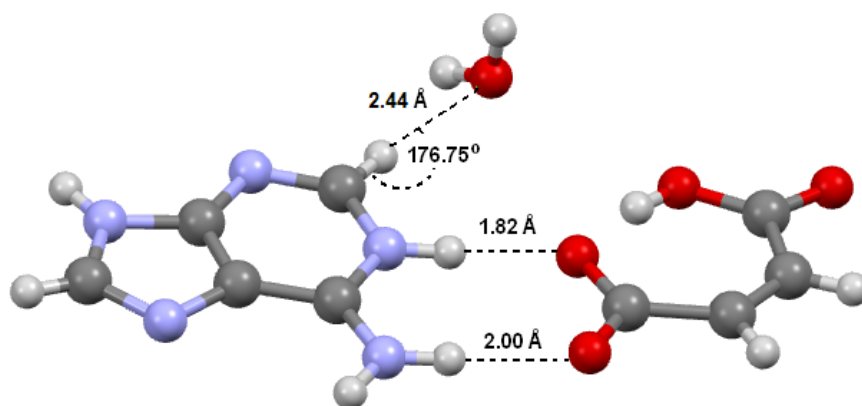


Fig. S1. View of RIGMIE crystal structure showing simultaneous interactions of positively charged nucleic basis with counter ion and with water molecule.

S. Sridhar and K. Ravikumar, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2007, **63**, o415-o418; CSD REFCODE: RIGMIE.